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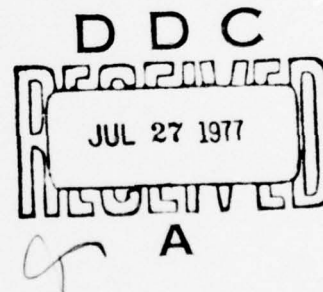
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THEORETICAL INVESTIGATION OF ANOMALOUS
PROPERTIES OF BCC Ti, Zr AND Hf ALLOYS

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D. de Fontaine
Principal Investigator

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20. approach based on Kikuchi's Cluster Variation method. The two methods of calculation for the self-diffusion coefficient of Zr give excellent agreement with experiment, the observed curvature of the Arrhenius plot being reproduced perfectly. Furthermore, diffusional anomalies observed in bcc-stabilized alloys of these metals and, in particular, the increase of the apparent activation energy with solute concentration are readily explained by the model. The phenomenological equations derived are simple to use, have straightforward physical content and may be employed to estimate diffusion coefficients in anomalous Group IV B transition metals and alloys when little experimental data is available.

1. FOREWORD (ABSTRACT)

A model for anomalous self-diffusion in the bcc-phase Group IV B transition metals, Ti, Zr and Hf is proposed. The model is based upon the identity of the activation complex for vacancy diffusion in the bcc lattice and the smallest unit (omega embryo) of a hexagonal phase, the omega phase, found in these metals and their alloys in a metastable state. The coefficient for self-diffusion is calculated as a function of temperature by means of a phenomenological expression for the free energy of formation of an omega embryo, and by means of a more fundamental approach based on Kikuchi's Cluster Variation method. The two methods of calculation for the self-diffusion coefficient of Zr give excellent agreement with experiment, the observed curvature of the Arrhenius plot being reproduced perfectly. Furthermore, diffusional anomalies observed in bcc-stabilized alloys of these metals and, in particular, the increase of the apparent activation energy with solute concentration are readily explained by the model. The phenomenological equations derived are simple to use, have straightforward physical content and may be employed to estimate diffusion coefficients in anomalous Group IV B transition metals and alloys when little experimental data is available.

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3. LIST OF ILLUSTRATIONS

- Figure 1: The configurations of the elementary ω embryo and the activated complex for diffusion. The atom at 0 exchanges place with a vacancy at V (a) by forming, in the process, an elementary ω embryo (b).
- Figure 2: Comparison of the diffusion coefficient predicted by the phenomenological model to the experimental data by Federer and Lundy⁽²⁰⁾.
- Figure 3: The concentration of ω embryos (activated complexes for diffusion) versus the absolute temperature. The concentration of ω embryos increases with a decrease in temperature as postulated in the phenomenological approach⁽¹⁵⁾.
- Figure 4: The diffusion coefficient predicted by the phenomenological approach is compared to the data of Murdock and Lundy⁽²³⁾ for self-diffusion (a), and to the data of Santos and Dymant⁽²⁴⁾ for diffusion of ^{44}Ti in Ti-Mn alloys of composition: (b) 9.7%Mn (c) 13.3%Mn, (d) 17.9%Mn and (e) 20.6%Mn.

4. BODY OF REPORT

4. 1. Introduction

The objective of this investigation was the search for a theoretical model for anomalous self-diffusion in the Group IV B transition metals: Titanium, Zirconium and Hafnium. These three metals, along with γ -Uranium and the rare earths δ -Cerium and β -Praseodymium exhibit anomalous diffusional properties^(1,2,3). Normal behavior is characterized by a diffusion coefficient D given by

$$D = D_0 \exp(-Q/RT)$$

with the pre-exponential factor D_0 of order 0.05 to $5.0 \text{ cm}^2/\text{sec}$ and activation energy given approximately by $Q = 34 T_m$ where T_m is the absolute temperature of melting and where R and T are the gas constant and absolute temperature respectively. D_0 and Q are approximately temperature independent since a plot of $\log D$ vs. $1/T$ yields a straight line over several decades of D . By contrast, the anomalous metals are characterized by significantly curved Arrhenius plots which have been interpreted as due either to a temperature variation of the activation energy or to the participation of more than one mechanism in bulk diffusion^(1,4).

Numerous attempts have been made to explain anomalous diffusion by means of two or more contributing mechanism^(1,4,5). This approach invariably encounters two serious difficulties:

the fact that anomalous diffusion is confined to a very specific group of metals is not explained nor can the values of the parameters for the low temperature mechanisms be rationalized: i.e., a pre-exponential factor which is several orders of magnitude lower than that of normal metals and an activation energy at least half as large as the high temperature one^(1,4).

The approach which allows for a temperature variation of the activation energy seemed to a few investigators to be a more sensible one^(4,6). Such a temperature dependence of Q is made plausible by the existence of a low temperature phase transition. Indeed, all anomalous metals present allotropic phase transitions; in particular Ti, Zr, Hf and Pr transform from bcc phase to the hexagonal close packed structure stable at low temperature, and the stable form of Uranium at room temperature is orthorhombic, a distorted hexagonal close-packed structure. In addition, Ti, Zr and Hf transform to a metastable hexagonal (but not close-packed) phase, the so-called omega phase, upon alloying⁽⁹⁾ or under pressure⁽¹⁰⁾. Furthermore, Ti, Zr, Ce and Hf are Group IV B elements, the transition metal counterparts of Group IV A elements, the light elements of which are covalently bonded. The trigonally bonded basal plane of the hexagonal ω structure has, in fact, the structure of the basal plane of graphite indicative of strong covalent component to the total binding energy.

Thus, the bcc structure appears to be a necessary but not sufficient condition for the diffusional anomalies, the additional condition required being that the bcc structure transform to a hexagonal phase at low temperature. Rather than seeking a connection between the anomalies and the hcp phase itself⁽⁶⁾, we attempted to establish the connection with the ω phase.

It can now be stated unequivocally that the objectives of the proposal research have been fully met:

1. a model which explains the experimental data has been found and gives excellent quantitative fit,
2. subsequent application of the model to self-diffusion in Ti alloys⁽¹¹⁾ has been equally successful,
3. our model is claimed by other investigators to be the most promising one to explain anomalous diffusion in certain bcc-phase rare earths⁽¹²⁾,
4. ours appears to be the only really new diffusion model proposed in the last 20 years. As such, it has prompted experimentalists^(13,14) to perform new measurements on the anomalous diffusers.

A brief summary of results obtained follows. Details will be found in the Ph.D Dissertation of Dr. J. M. Sanchez⁽¹¹⁾ and in relevant publications⁽¹⁵⁻¹⁷⁾.

4.2. Diffraction Model

Our first task, before tackling the difficult one of the diffusion mechanism, was to understand better the ω phase transformation. We therefore attempted to explain electron and neutron diffraction patterns from bcc Ti and Zr alloys transforming to the ω phase. It was found essential to include anharmonic effects in both the free energy and the diffraction equations. In this way, we were able to establish a direct connection between a Landau expression for the free energy of the transforming bcc phase and the diffraction pattern. Direct Fourier and optical transforms yielded a plausible picture of patterns of atomic displacements, and comparison with neutron diffraction data⁽¹⁸⁾ yielded a plausible temperature dependence of the third order anharmonic free energy term $B(T)$ to be used in the diffusion model. Details are to be found in Ref. 16.

4.3. Phenomenological Model

From the start, we assumed a vacancy mechanism, i.e., a diffusing atom exchanging places with a vacant substitutional site. In so doing, the atom passes through an unstable saddle point configuration, momentarily forming an "activated complex" which spontaneously decays.

The key to the explanation of anomalous diffusion consists of recognizing that, in bcc structures, the required activated complex is none other than an ω embryo, that is, the smallest unit or cluster of neighboring atoms having the essential ω -structure characteristics. This can be seen in Figure 1: The top portion (a) shows a (111) plane ABC and an atom at O occupying the normal body-centered site just below the ABC triangle. For this atom to exchange places with a nearest-neighbor vacancy at V, it must first pass through the "activated" position within and at the center of the ABC triangle. This activated configuration is shown in Figure 1 (b), which is an ω embryo exhibiting elementary "collapse" of two neighboring (111) planes, the one at ABC and the one at O. One recognizes in Figure 1 (b) the characteristic trigonally bonded ω structure⁽⁸⁾. Once the configuration depicted in Figure 1 (b) is reached, the central atom will jump to a nearest neighbor vacancy, if available, without any extra expenditure in energy as in the case of normal diffusion. The essential difference with normal diffusion comes about when the re-

versible work of formation of the activated state is calculated. In the case of systems in which the ω structure is a low temperature metastable phase, close to the transition temperature the free energy of formation of an activated complex (or ω embryo) will be much smaller than in the case of normal bcc metals, resulting in a higher concentration of activated states and consequently enhancing diffusion at low temperatures. On the other hand, in the limit of high temperatures, random thermal vibrations will tend to destroy the ω embryos and the diffusion process should be characterized by normal values and behavior of the diffusion coefficient.

By making the assumption that the free energy change in forming unit amount of ω is described by a Landau expansion with third-order coefficient given by

$$B(T) \approx \text{Const.}/T \quad (1)$$

it is possible to derive the following expression for the coefficient of self-diffusion

$$D = D_0 \exp(-Q/RT) \exp(\Delta H_m T_0 / RT^2) \quad (2)$$

in which D_0 is the usual preexponential factor, Q is the usual activation energy, estimated here by the "normal" rule $Q = 34 T_m$ where T_m is the melting temperature. ΔH_m is the motion enthalpy for vacancy diffusion and T_0 is the bcc $\rightarrow \omega$ transition temperature.

In the particular case of self-diffusion in bcc Zr, Q is 70 kcal/mole, and T_0 is estimated to be about 890°K by extrapolation of the ω transition temperature curve vs. composition in a Zr-Nb alloy⁽¹⁹⁾. The remaining two parameters D_0 and ΔH_m can be determined by fitting Equation (2) to the data of Federer and Lundy⁽²⁰⁾ yielding $D_0 = 0.21 \text{ cm}^2/\text{sec}$ and $\Delta H_m = 32.5 \text{ kcal/mole}$, both parameters falling well within the expected range of values. As can be seen from Figure 2, the fit is as perfect as the data warrants. Additional details are given in Reference 15.

4.4. Cluster Variation Model

The temperature dependence given in Equation (1) was merely postulated; it was thus desired to obtain a more fundamental justification thereof. To that end, the free energy of the bcc phase was written as a function of cluster frequencies, the largest cluster consisting of the 8-point primitive bcc unit cell, each point being occupied by a 0, +1 or -1 displacement (on a suitable scale) along a given [111] direction. It was thus possible to simulate activated complexes or other intermediate structure between perfect bcc and perfect ω . The internal energy was taken as a linear combination of cluster frequencies and the entropy was derived by the Cluster Variation method of Kikuchi⁽²¹⁾.

At any temperature, equilibrium states are obtained by minimizing the free energy with respect to cluster frequencies. This is a formidable task since there are $3^8 = 6561$ cluster variables (not all distinct), and the same number of simultaneous non-linear algebraic equations to be solved. Dr. Sanchez was able to do this by modifying the Natural Iteration algorithm recently developed by Kikuchi⁽²²⁾. It was then possible to calculate directly the temperature dependence of activated complexes, as shown in Figure 3. From there, it was possible, as was done above, to obtain the temperature dependence of the diffusion coefficient for the case of pure Zr. The fit to the data by this method was every bit as good as that shown in Fig. 2, but this time with a solid

justification for all temperature dependences. In addition to providing new insight into the ω phase transformation, this study provided additional returns: (a) it was apparently the first application of the cluster variation method (CVM) to displacive transitions, perhaps paving the way for future use of the CVM to this important field of phase transformations; (b) it was the most ambitious CVM calculation yet undertaken, in terms of number of variables and equations, thereby demonstrating the feasibility of solving very complex problems by the algorithms developed. From the strictly computational viewpoint, the experience gained has been invaluable for our new ARO(D)-sponsored project which has just gotten under way.

A complete treatment of the problem will be found in the Ph.D Dissertation of Dr. Sanchez⁽¹¹⁾ and in forthcoming publications⁽¹⁷⁾.

4.5. Solvent Diffusion

Group IV B transition metals with β -stabilizing alloying additions do not conform to well-established rules for solvent diffusion: normally, if an alloying addition lowers the solidus temperature T_m , a corresponding lowering of the activation energy for diffusion takes place as expected from the relation $Q \approx 34 T_m$. In the anomalous metals, however, the effect of β -stabilizing elements appears to be the exact opposite: alloying additions which lower the solidus temperature result in an increase in the activation energy for diffusion. For instance, solvent diffusion in Ti-rich Ti-V alloys is "anomalous", with activation energy increasing with V content, while V-rich alloys behave normally. Recent experiments on diffusion of ^{44}Ti in Ti-Mn and Ti-Co alloys⁽²⁴⁾ indicate that the curvature of the Arrhenius plot decreases as the alloying element content is increased. Also if the data is analyzed in terms of a best straight-line fit, both effective D_0 and Q values are found to be anomalously low in Mn or Co-lean alloys, to become progressively more normal as the alloying element content is increased.

Such behaviour, which defies interpretation in terms of a normal diffusion process, is readily explained in terms of the ω -embryo mechanism. Since Mn(or Co) is a β -stabilizing element, the $\beta \rightarrow \omega$ transition temperature T_0 decreases rapidly with alloying additions, more rapidly in fact than the solidus temperature T_m . This means that, at a given temperature, increased alloying effectively take the system further away from the

ω transition so that, by Figure 3, the concentration of ω -embryos is expected to decrease, resulting in increasingly "normal" behaviour.

The phenomenological model presented in Section 3 is particularly convenient for analyzing these effects quantitatively. By consideration of Equation (2), we may define an effective temperature-dependent activation energy

$$Q_{\text{eff}}(T,c) \cong 34 T_m(c) \left[1 - \alpha \frac{T_0(c)}{T} \right] \quad (3)$$

where α is a constant of the order of 0.5, and where both solidus and $\beta \rightarrow \omega$ transition temperatures T_m and T_0 are concentration dependent. Application of Equation (3) to the Ti-Mn system result in the calculated curves shown in Figures 4 a-e. Not only is the fit to the data as good as can be expected, but the resulting values of the fitted parameters fall well within the allowed ranges, while the curvature of the Arrhenius plots decreases as the transition temperature T_0 decreases with concentration c . Hence, it can be concluded that all anomalies have been explained satisfactorily.

Additional details are given in the Ph.D Dissertation of Dr. Sanchez⁽¹¹⁾ and in forthcoming publications⁽¹⁷⁾.

4.6. Conclusion

The proposed model is a simple one, with clear qualitative physical interpretation and excellent quantitative fit to experimental data. By relating the diffusional anomalies of Ti, Zr and Hf metals and alloys to the important ω displacive transition, we have discovered a new diffusional model, surely a significant accomplishment in its own right. Already, our model is cited in very recent review articles^(25,26), and is described as "very convincing".

From a practical point of view, the model is found to have predictive value: Equations (2) or (3) are sufficiently simple, and most parameters can be approximated well enough to enable an experimenter to predict the diffusional properties of an anomalous system for various temperatures and concentrations, without the necessity of performing costly and time-consuming experiments. For example, resistance to high-temperature steady-state creep in Ti alloys can be significantly improved by adding β -stabilizing elements, and by avoiding hcp-stabilizing elements such as Al. The analysis can be made quantitative through the use of Equation (3).

Much work of a fundamental nature remains to be done. Here are a few suggestions:

- a. better analytical treatments of the ω phase transformation are required, either in the framework of the displacive wave method

with anharmonic terms in the free energy, or by the Cluster Variation method with larger clusters than the ones used here.

- b. the best quantitative experimental knowledge of the ω transformation is obtained by diffraction methods: X-ray, electron, and particularly neutron diffraction. Much more work is needed to collect data over a range of concentrations and temperatures in a variety of Ti, Zr and Hf alloys, and in various bcc-based ordered alloys such as β -CuZn⁽²⁷⁾.
- c. Since the ω phase is found to be stable in the pure elements at high pressure, experiments of both diffraction and diffusion types should be conducted under pressure in Ti and Zr alloys as a function of average concentration and temperature.
- d. other anomalous metals such as bcc Ce should be investigated in the light of the proposed model for Ti, Zr and Hf. In particular, it would be interesting to find out whether high-pressure or high-alloy content metastable phases with structure similar to ω exist for these rare earths. Such studies have not been conducted presumably because these elements are very reactive and present only a very narrow temperature range for the high-temperature bcc phases.
- e. anomalous diffusion should be further investigated, in both element and alloy, by such techniques as the isotope effect, as is currently being performed by Professor Lazarus and co-workers. Early results

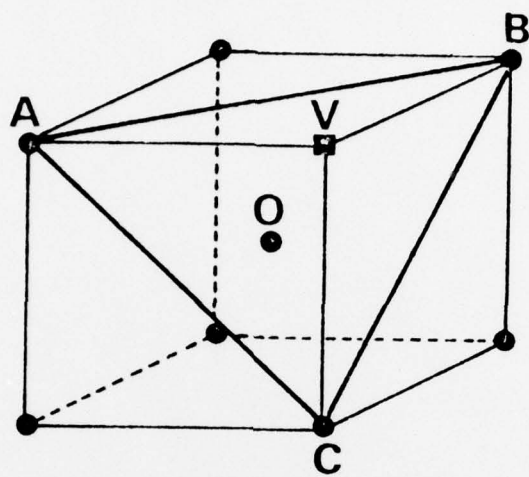
appear to substantiate our model⁽¹⁴⁾.

In the past, the discovery of a new theoretical model has often suggested renewed experimental activity in the field, while providing useful guidelines for practical applications. We believe that this will also occur in the present instance if appropriate funding is available.

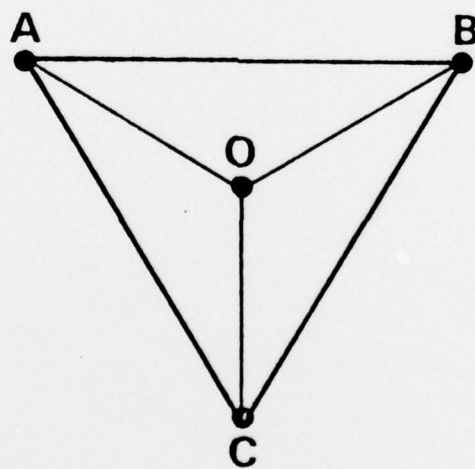
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(a)



(b)

FIG. 1

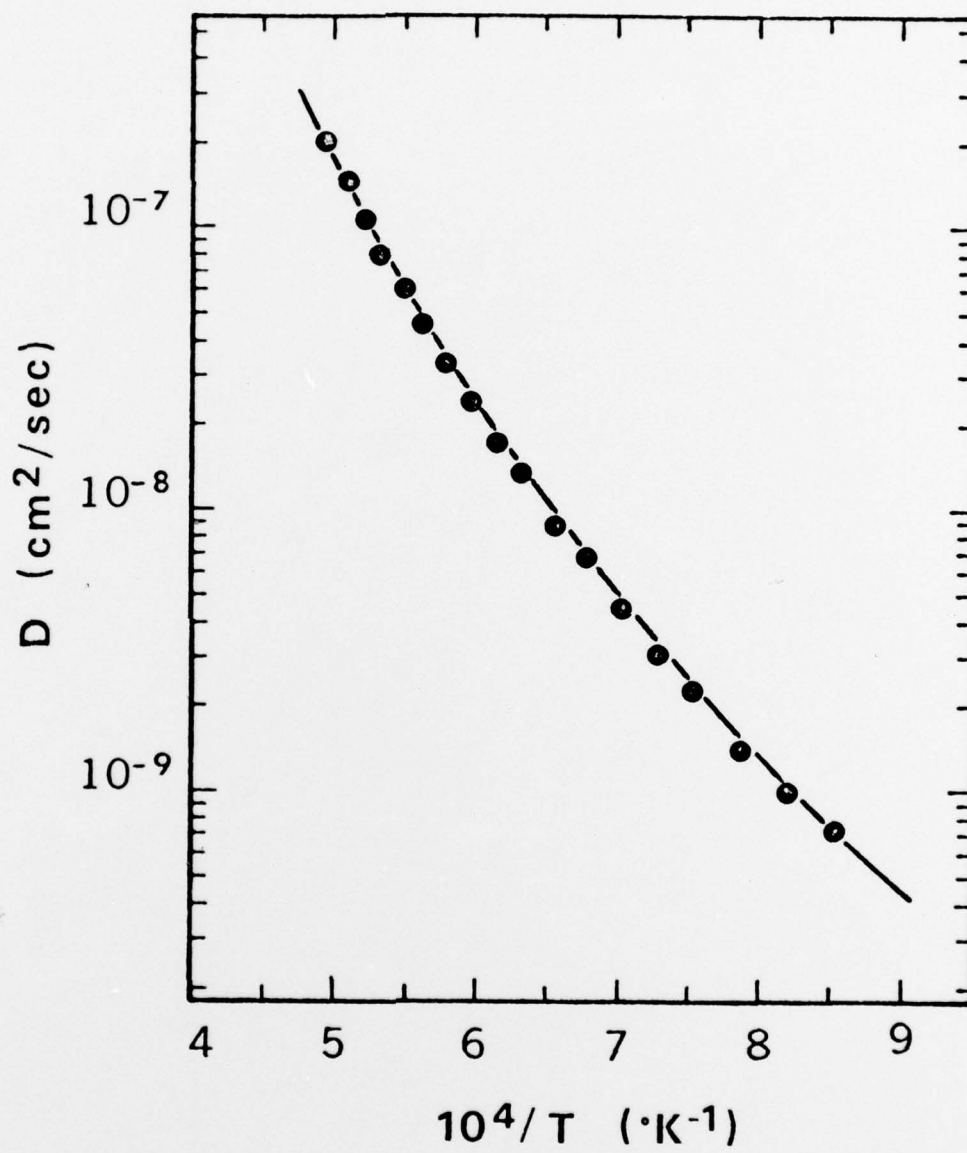


FIG. 2

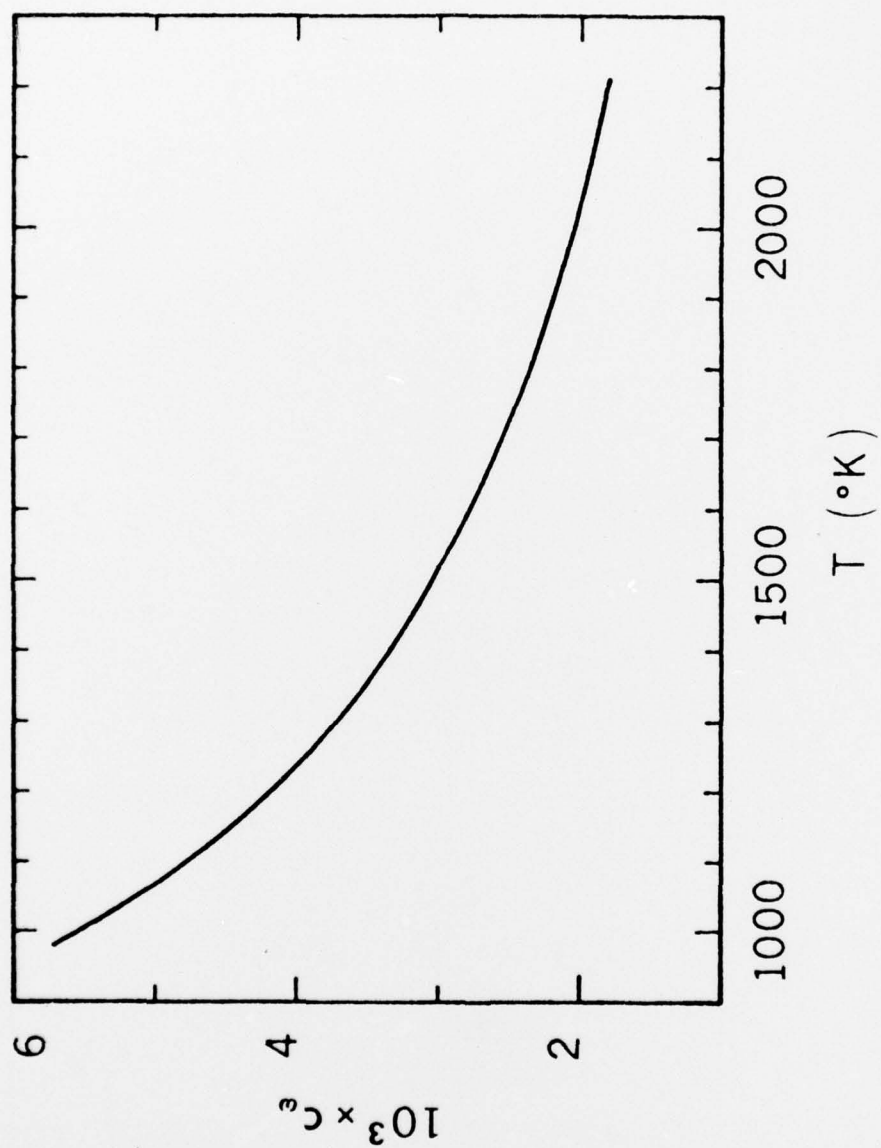


FIG. 3

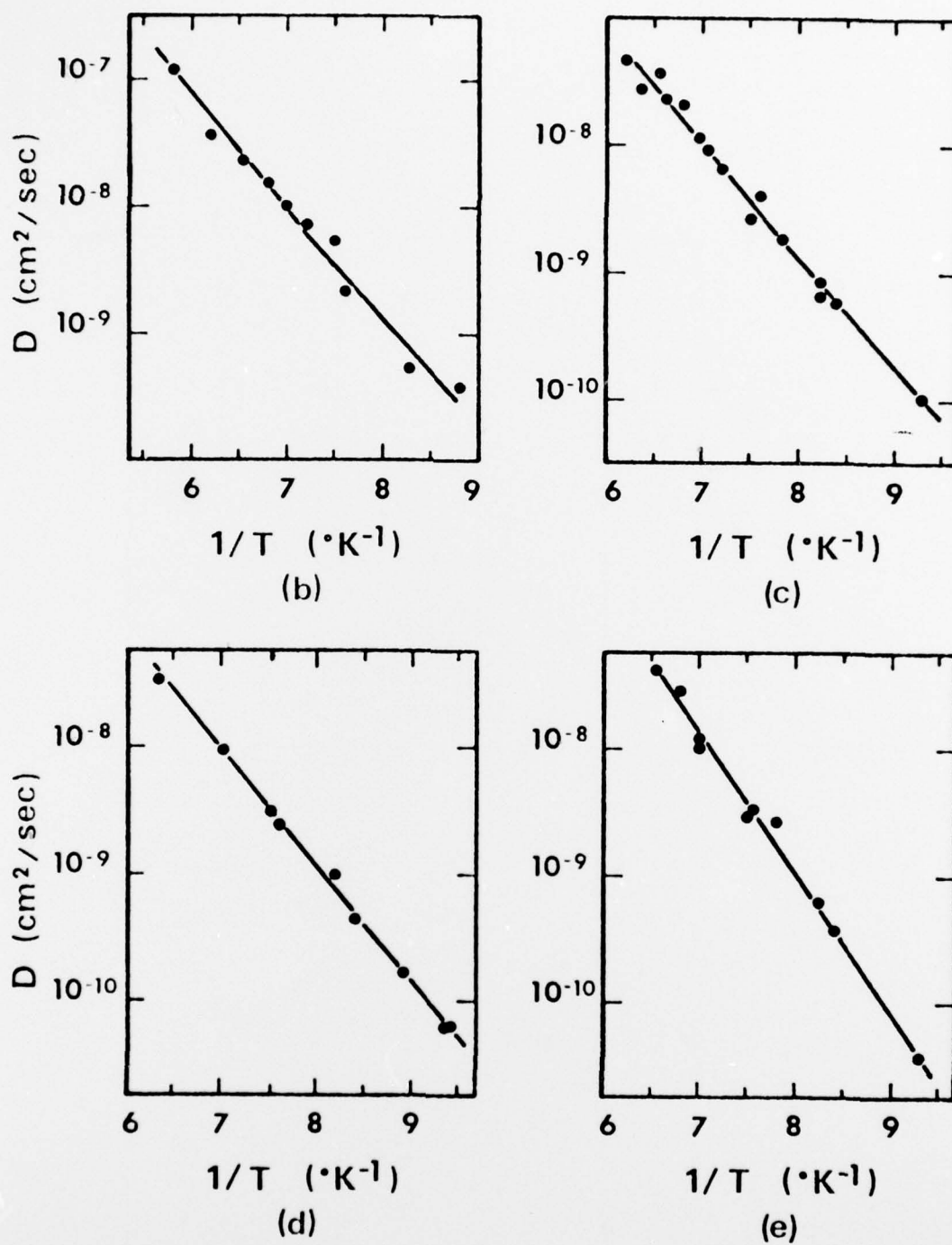


FIG. 4

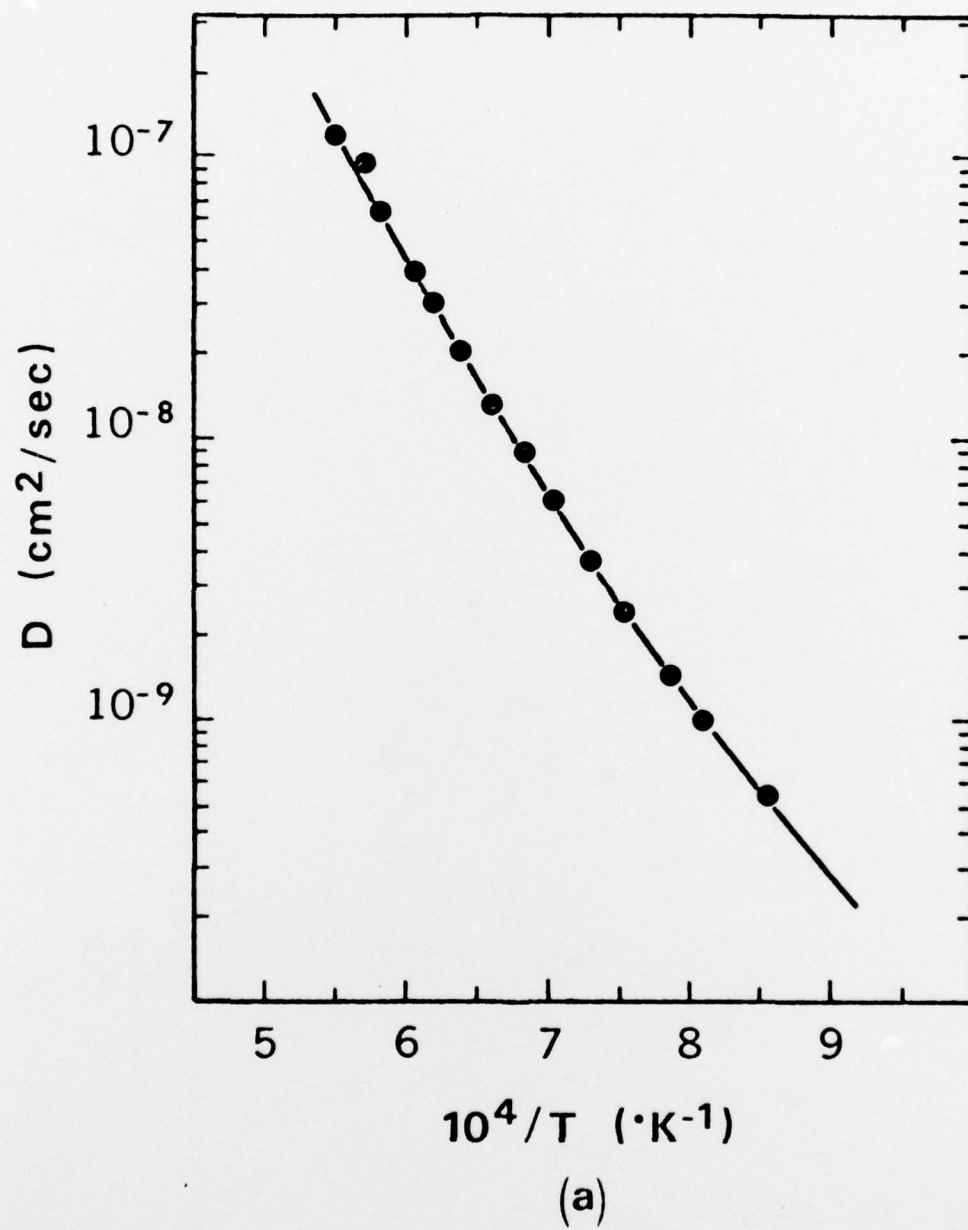


FIG. 5

APPENDIX

6. THESES, PUBLICATIONS, PRESENTATIONS6.1. Ph.D Thesis

Dr. J.M. Sanchez (Thesis Committee Chairman: D. de Fontaine)
Model for Anomalous Diffusion in the Group IV B
Transition Metals. UCLA School of Engineering and
Applied Science, Los Angeles, CA, 90024, April 1977.

6.2. Publications

Dr. J.M. Sanchez and D. de Fontaine, Physical Review Letters,
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Dr. J.M. Sanchez and D. de Fontaine, Journal of Applied
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6.3. Oral Presentations

Sanchez, J.M. and de Fontaine, D., "A Structural Model for
the Omega Phase Transformation", General meeting
of the American Physical Society, Anaheim, CA,
January 29, 1975.

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the Omega Phase Transformation, TMS-AIME Spring
Meeting, Toronto, Canada, May 22, 1975.

Sanchez, J.M. and de Fontaine, D., "Anomalous Self-Diffusion
in Omega-Forming Transition Metals," AIME Meeting,
Las Vegas, Nevada, February 24, 1976.

de Fontaine, D. and Sanchez, J.M., "Structural Model for
the Omega Phase Transformation", American Crystal-
lographic Association Summer Meeting, Northwestern
University, Evanston, Illinois, August 10, 1976.

Sanchez, J.M. and de Fontaine, D., "Anomalous Self-Diffusion
and the Omega Phase Transformation", TMS-Meeting,
Atlanta, Georgia, March 9, 1977.

Sanchez, J.M. and de Fontaine, D., "The Omega Phase Trans-
formation and its Effect on Anomalous Diffusion",
American Physical Society Meeting, San Diego, CA,
March 21, 1977.